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LOW-DISCREPANCY POINT SETS IN TRANSPORT CODES

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ABSTRACT

A drawback to Monte Carlo methods of computation is its rate of convergence. There are methods of sampling that have a better error estimate than those using random numbers. This paper gives the result of some preliminary experiments with these sampling methods on two neutron transport problems.

LOW-DISCREPANCY POINT SETS IN TRANSPORT CODES

The Monte Carlo method is useful in solving a variety of problems such as: the evaluation of multiple integrals, the solution of linear equations, the simulation of particle transport, and the simulation of thermodynamical systems. The only drawback to Monte Carlo computations is its rather slow rate of convergence, that is, the estimated error depends on $1/\text{SQRT}(N)$ where N is the number of trials made.

There are methods of sampling which have a better error estimate.¹ These methods have been used for multidimensional integrational, but they have not found much application in other areas. This paper gives the results of some experiments with these sampling methods on neutron transport problems.

One measure of the sampling efficiency of a set of points is the discrepancy. Fig. 1. illustrates the idea in two dimensions. The local discrepancy of a point (x,y) in the unit square is given by the expression:

$$g(x,y) = V(x,y)/N - xy$$

where

$V(x,y)$ = the number of points inside the rectangle extending from the origin to the point (x,y) .

A global measure of the unevenness of the points can be given by a norm of $g(x,y)$ taken over the unit square. A random sequence has discrepancy proportional to $1/\text{SQRT}(N)$. There exist sets of points, called quasi-random, with discrepancy lower than this. There are methods of sampling which have a better error estimate. Two such sequences are used in these experiments. Figure 2 shows the difference in a random sequence (from a random number generator) and a quasi-random sequence. An intuitive appreciation for the increased efficiency of the quasi-random sequence can be obtained from Figs. 3-6. Figure 3 shows one point with lines parallel to the coordinate axes drawn through it. These lines divide the square into four rectangles. A random sequence would put the next point in a given rectangle with a probability proportional to the area of the rectangle. A quasi-random sequence always puts the next point in the biggest (or one of the biggest if there are several) rectangles. This effect is shown in Figs. 4-6.

As quasi-random sequences are more complicated to compute than pseudorandom sequences, it is not easy to use them in a general purpose Monte Carlo transport code. These sequences may be used for generating source parameters with-

out much overhead, however. A version of the code MNCP² was used with the source distributions generated with quasi-random sequences. Two problems were run as a computational experiment.

The first problem is shown in Fig. 7. It is a bent concrete pipe with a 14 MeV isotropic neutron source in one end. The quantity measured was the flux through the other end. On this problem, not much difference could be seen between the runs with a random number generator and those with the quasi-random sequences. Figures 8-10 show plots of the mean, relative error, and figure-of-merit vs the number of particles run using a random number generator. (the figure-of-merit is defined to be the reciprocal of the sample variance times the time used. For a truly random process, this number should be constant.) The corresponding graphs are shown for two different quasi-random sequences used for source sampling in Figs. 11-16. There is not much difference among the graphs at least showing that the quasi-random sequences do not cause trouble with a well-behaved problem.

The second problem is shown in Fig. 17. The object is a top-hat shaped structure of concrete. The (not very realistic) densities are 10 g/cc and 20 g/cc in the bottom and top central cylinders, respectively. The first lower ring has a density of .5 g/cc and the outer ring 2 g/cc. The upper cylinder is ringed by a void. A 14 MeV isotropic neutron source is placed at the bottom of the object and the flux through the top central surface is measured.

Figure 18 shows the mean flux through the top cylinder plotted vs the number of particles using a random number generator for the source sampling. When 65,000 particles were run, the mean began to increase to about 10% of its apparently stable value. The plot of estimated error, Fig. 19, shows the error suddenly doubling. The figure-of-merit plot in Fig. 20 is even more striking, showing a collapse in reliability around 70,000 particles.

Using one of the quasi-random sequences, Figs. 21-23 were obtained. The collapse in the figure-of-merit happens about 20,000 points (Fig. 23.) It seems that whatever caused the instability of the problem was exposed much sooner by using the quasi-random points. The relative error seems better than that using the random number generator but the small figure-of-merit indicates that neither result is extremely reliable.

Another quasi-random sequence was tried giving the results shown in Figs. 24-26. The sequence has some well-known structure and this is reflected in the results. Still, the collapse of the figure-of-merit happens around 10,000 particles rather than around 70,000 as with the random sequence.

On the basis of these experiments, it seems that using quasi-random sequences do not introduce any new problems into transport computations; however, they can be useful in guarding against "bad luck" as in the second problem.

The first sequence used is defined by taking the Nth point as the fractional part of $N\sqrt{2}$ for the X coordinate and the fractional part of $N\sqrt{3}$ for the Y coordinate.

The second sequence is based on the Halton sequence.³ Some modifications based on the ideas of.⁴ For a prime P, define S(P) to be the nearest integer to P times the fractional part of \sqrt{P} . The Nth term of the sequence is given by the prescription:

1. Write N in base P.
2. Reverse the P-ary digits.
3. Multiply each digit (modulo P) by S(P).
4. Treat the result as a base P fraction.

REFERENCES

1. Niederreiter, H., Quasi-Monte Carlo Method and Pseudo-Random Numbers, Bull. Am. Math. Soc., 84, (1978), 957-1041.
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3. Halton, J.H., On the Efficiency of Certain Quasi-random Sequences in Evaluating Multi-dimensional Integrals, Numer. Math. 2(1960), 84-90.
4. Warnock, T. T., Computational Investigations of Low-discrepancy Point Sets. Applications of Number Theory to Numerical Analysis (S. K. Zaremba, ed.), Academic Press, New York 1972, pp. 319-343.

FIGURE 1
DISCREPANCY

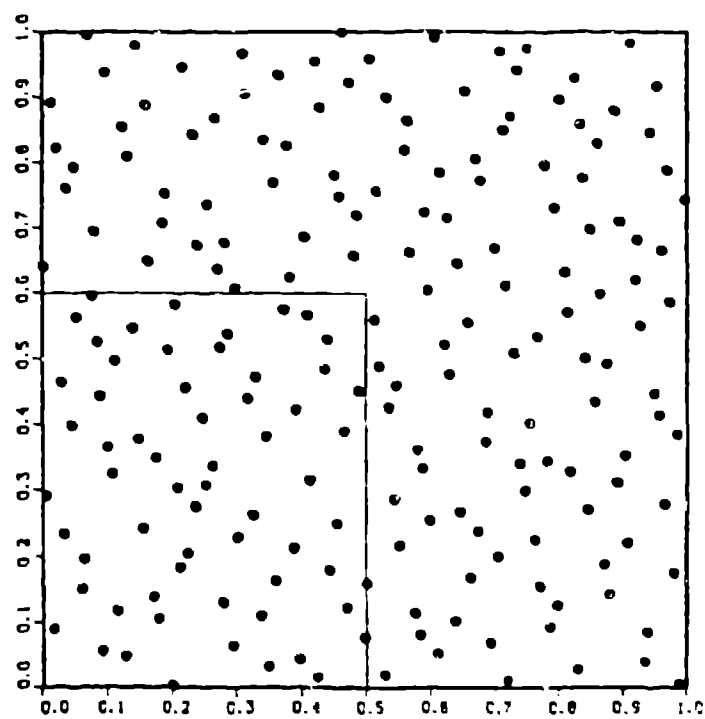
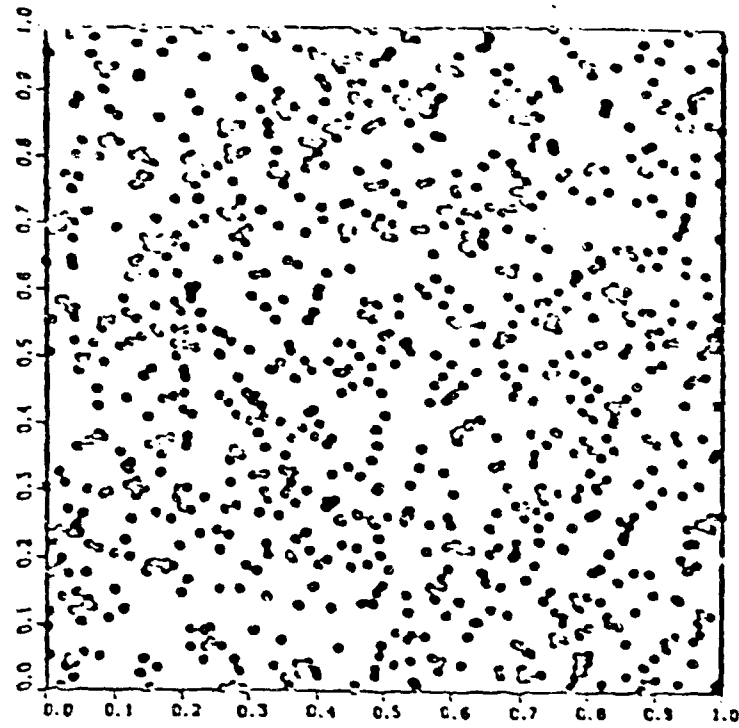


FIGURE 2
PSEUDO-RANDOM



RADICAL INVERSE

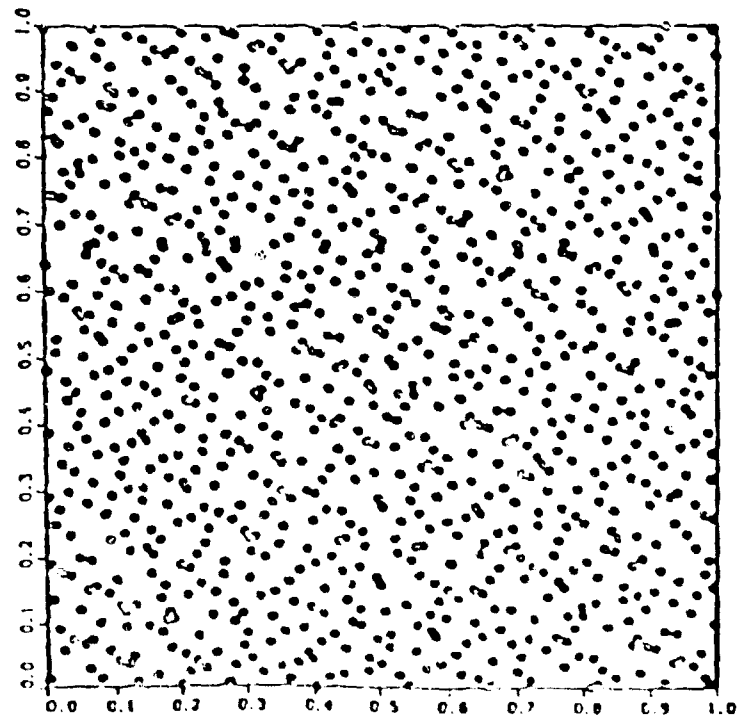


FIGURE 3
RADICAL INVERSE

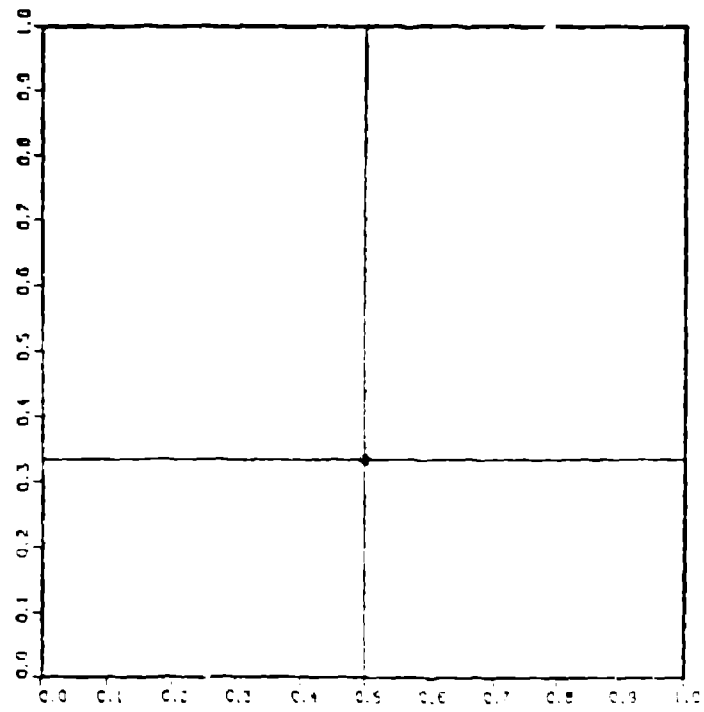


FIGURE 4
RADICAL INVERSE

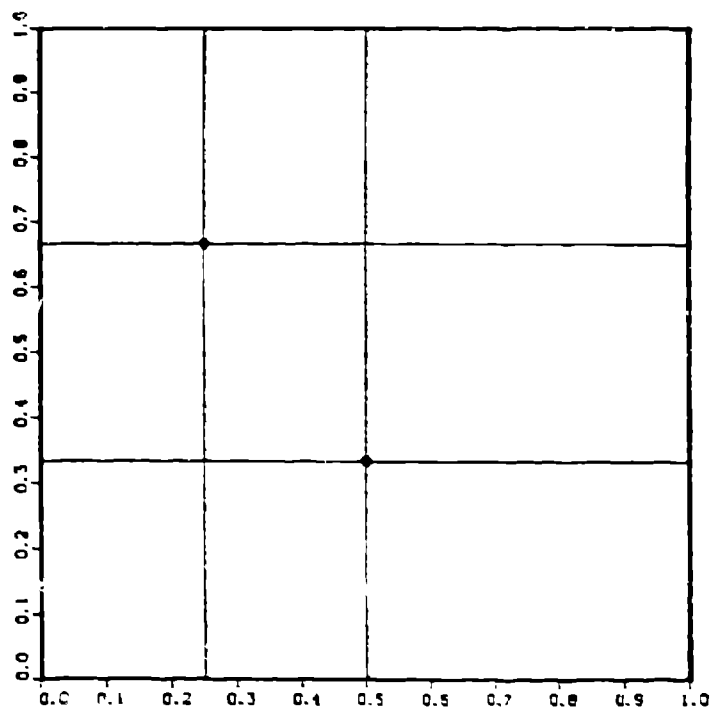


FIGURE 5
RADICAL INVERSE

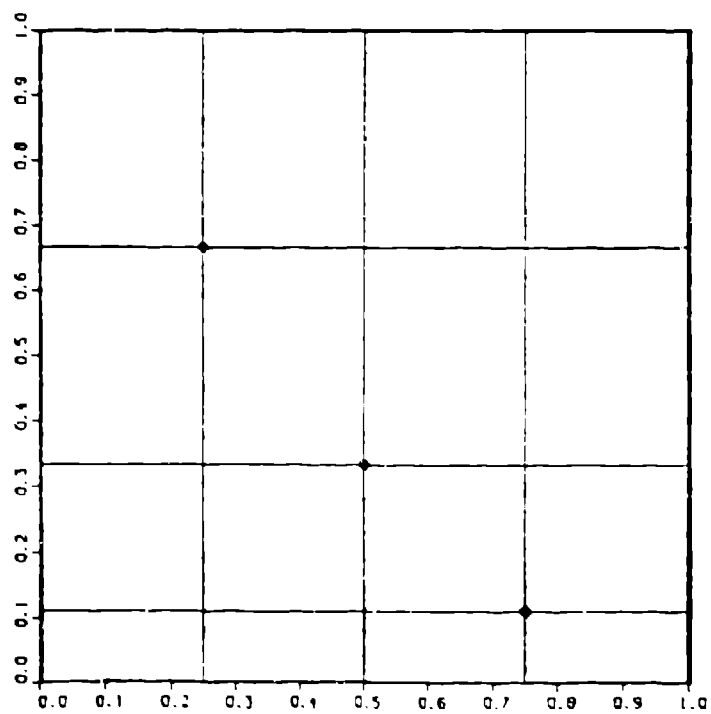
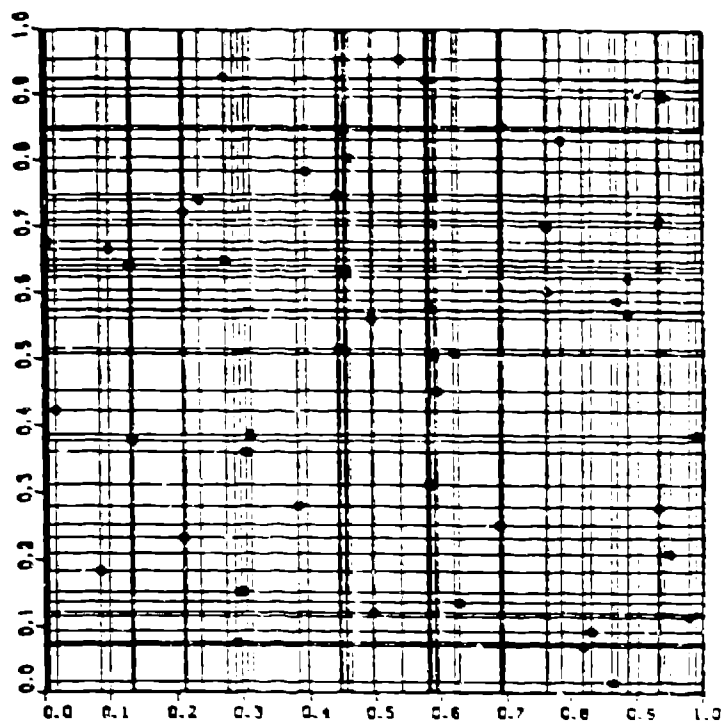


FIGURE 6
PSEUDO-RANDOM



RADICAL INVERSE

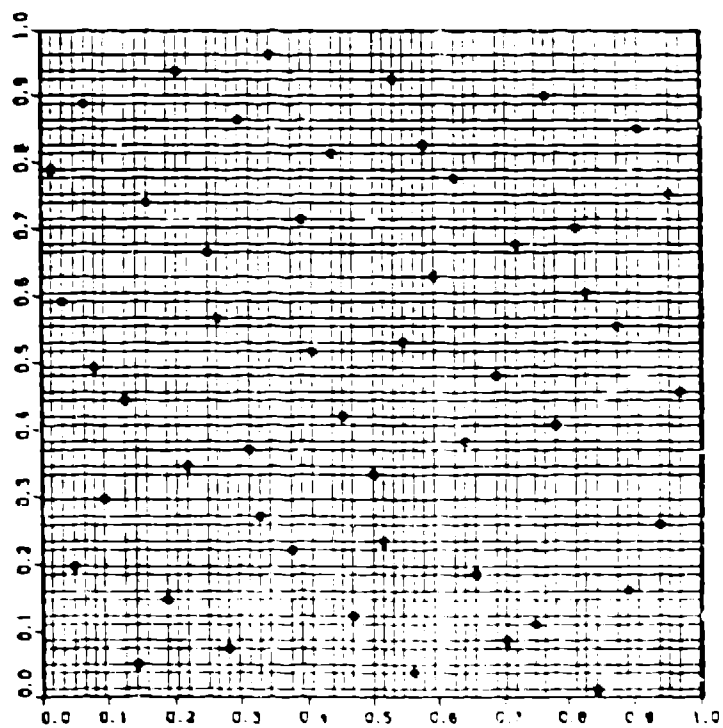


FIGURE 7

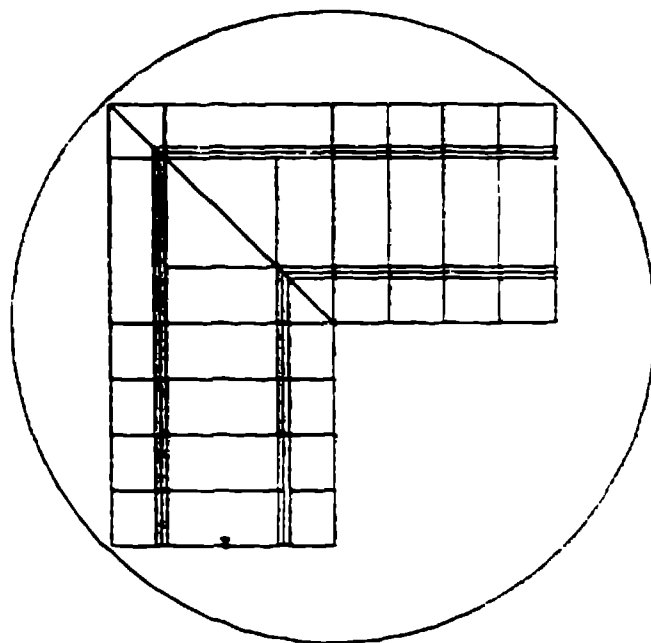
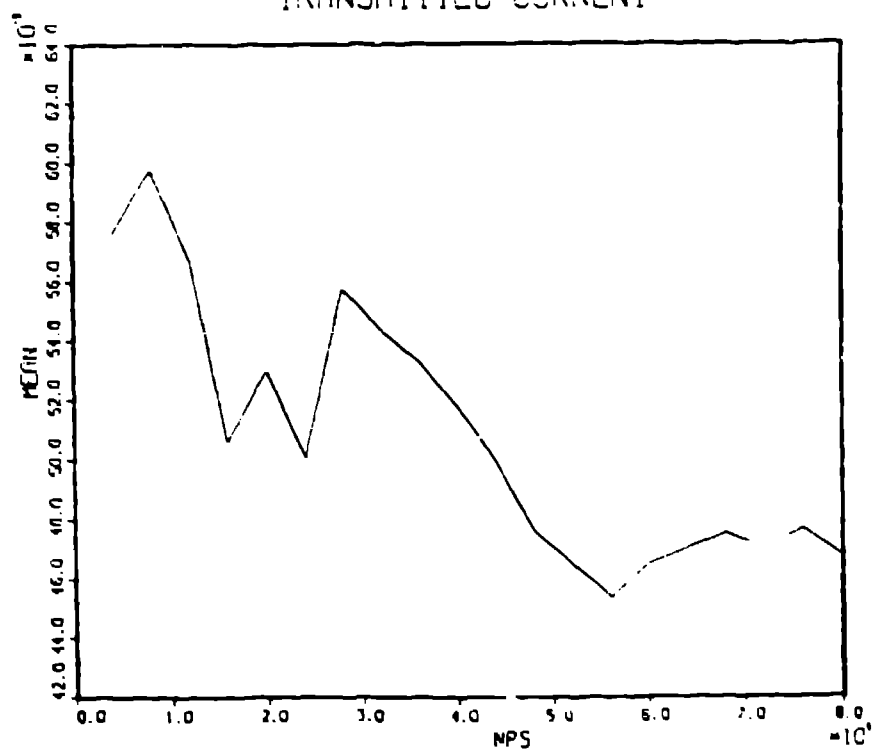
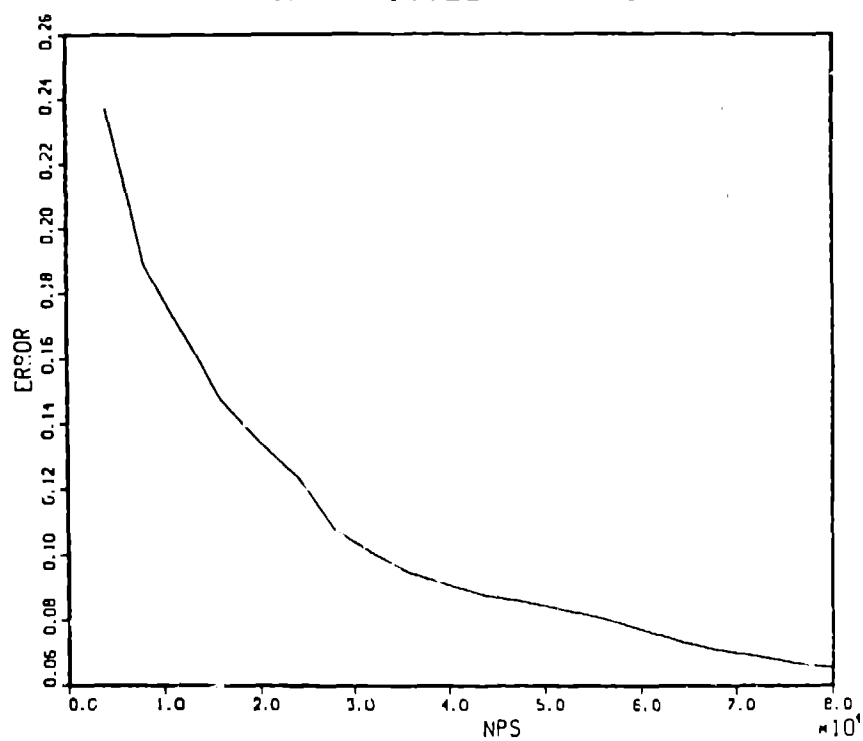


FIGURE 8
TRANSMITTED CURRENT



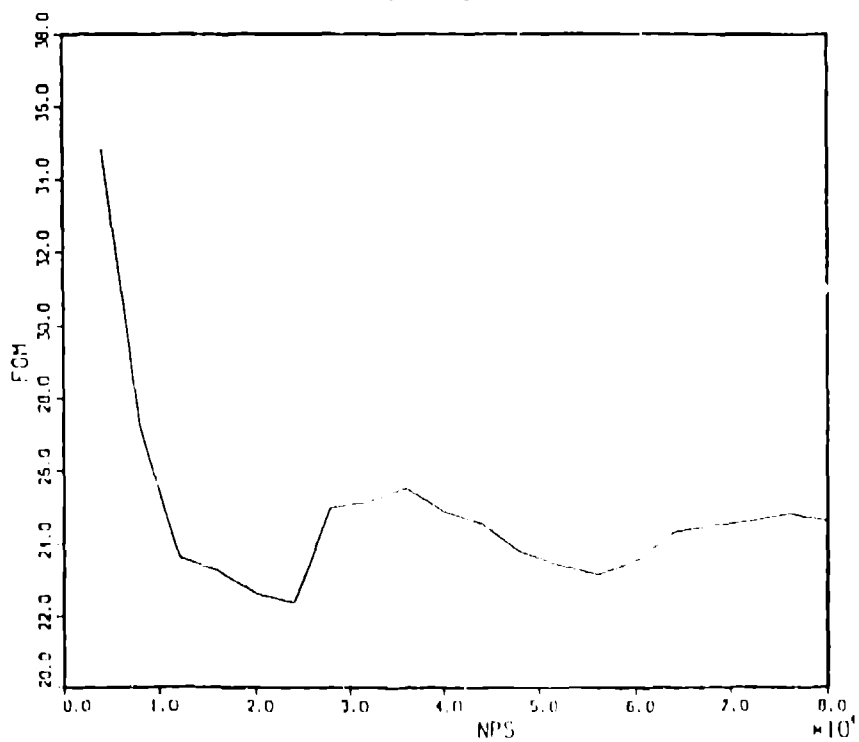
PCNP 28 03/12/82
Y 03/12/82 11:32:06
TITLE-
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
M MULT 1
C COSINE 2
E ENERGY 100
T TIME 1
DUMP DUMP 2
—— RUNTPE

FIGURE 9
TRANSMITTED CURRENT



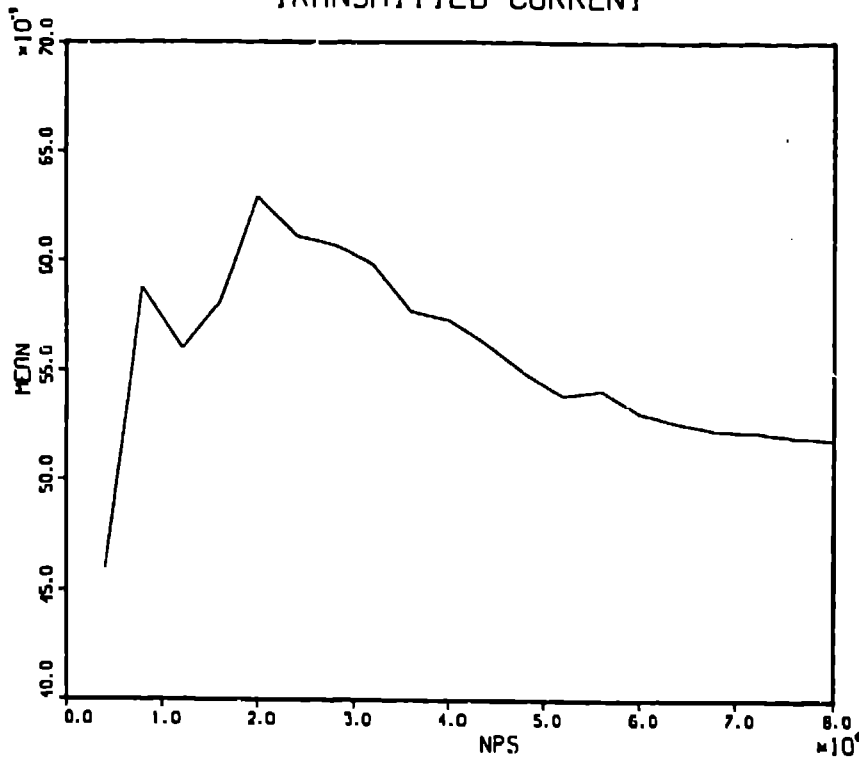
MCNP 28 03/12/82
Y 03/12/821113210G
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
H MULT 1
C COSINE 2
E ENERGY 111
T TIME 1
DUMP DUMP 2
—— RUNTPE

FIGURE 10
TRANSMITTED CURRENT



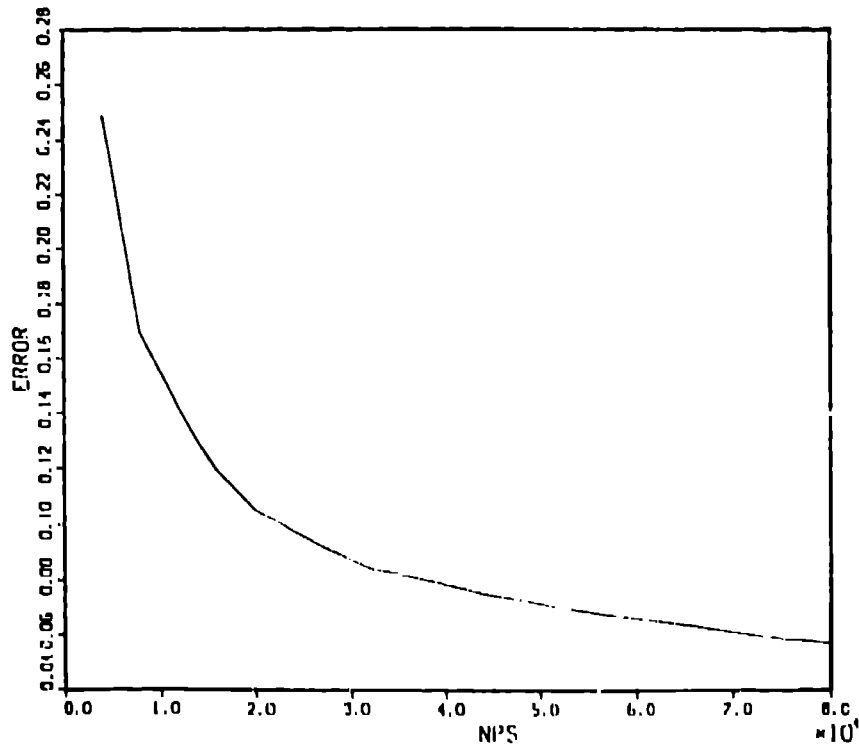
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Y 03/12/821113210G
TALLY 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
H MULT 1
C COSINE 2
E ENERGY 111
T TIME 1
DUMP DUMP 2
—— RUNTPE

FIGURE 11
TRANSMITTED CURRENT



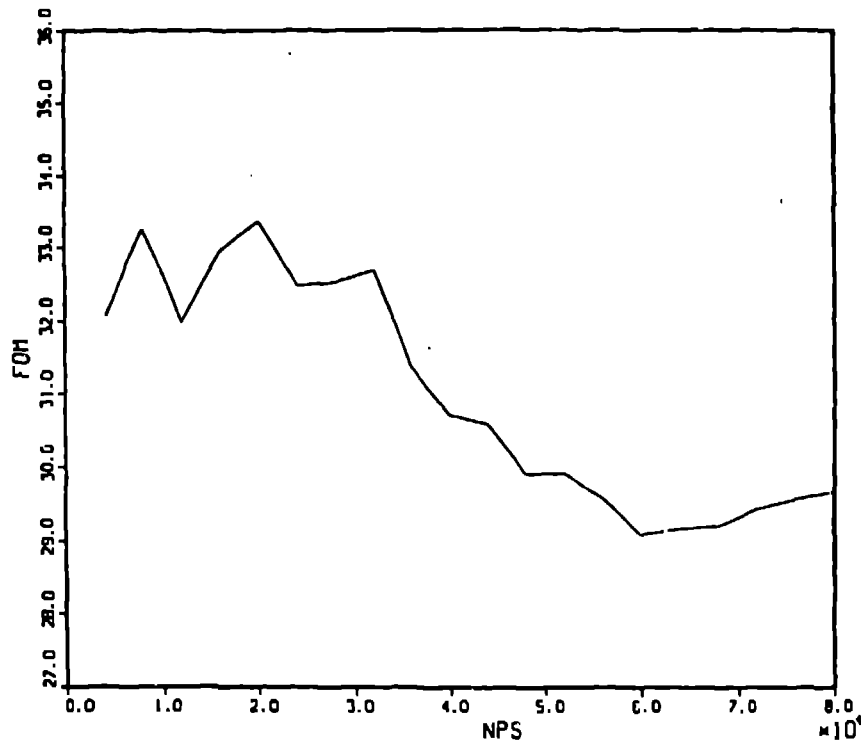
MCNP 28 03/15/82
Y 03/15/8210:34:45
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
H MULT 1
C COSINE 2
E ENERGY 117
T TIME 1
DUMP DUMP 2
----- RUNTPE

FIGURE 12
TRANSMITTED CURRENT



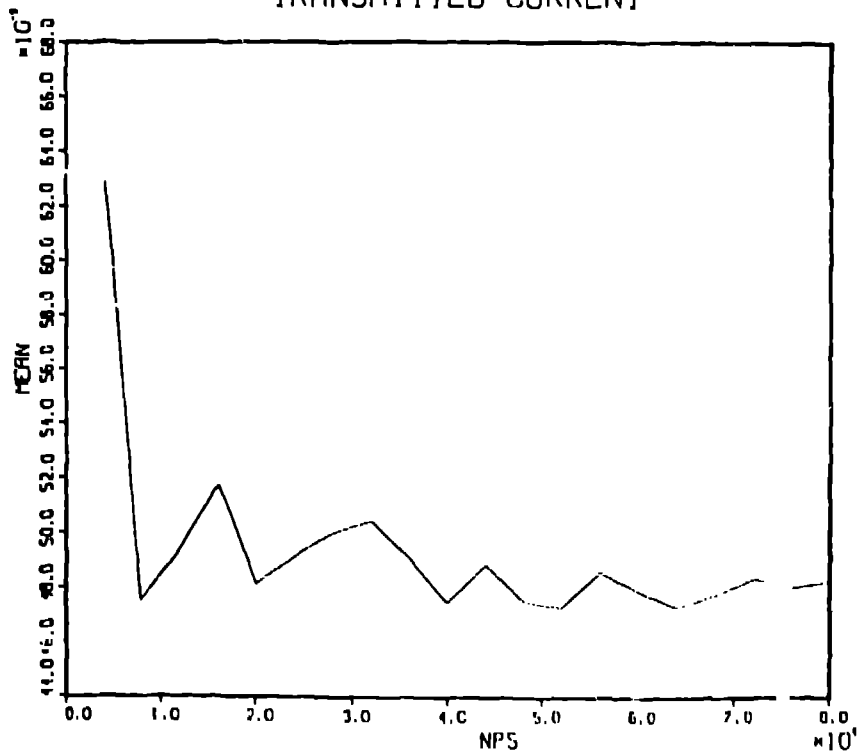
MCNP 28 03/15/82
Y 03/15/8210:34:45
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
H MULT 1
C COSINE 2
E ENERGY 117
T TIME 1
DUMP DUMP 2
----- RUNTPE

FIGURE 13
TRANSMITTED CURRENT



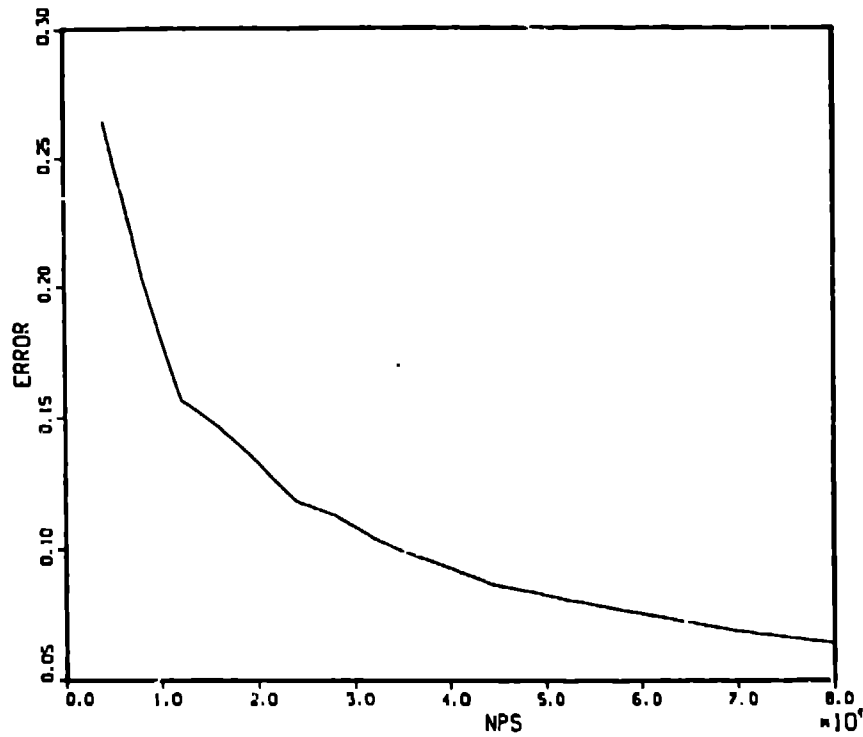
MCNP 28 03/15/82
Y 03/15/82 0:34:45
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
H MULT 1
C COSINE 2
E ENERGY 117
T TIME 1
DUMP DUMP 2
— RUNTPE

FIGURE 14
TRANSMITTED CURRENT



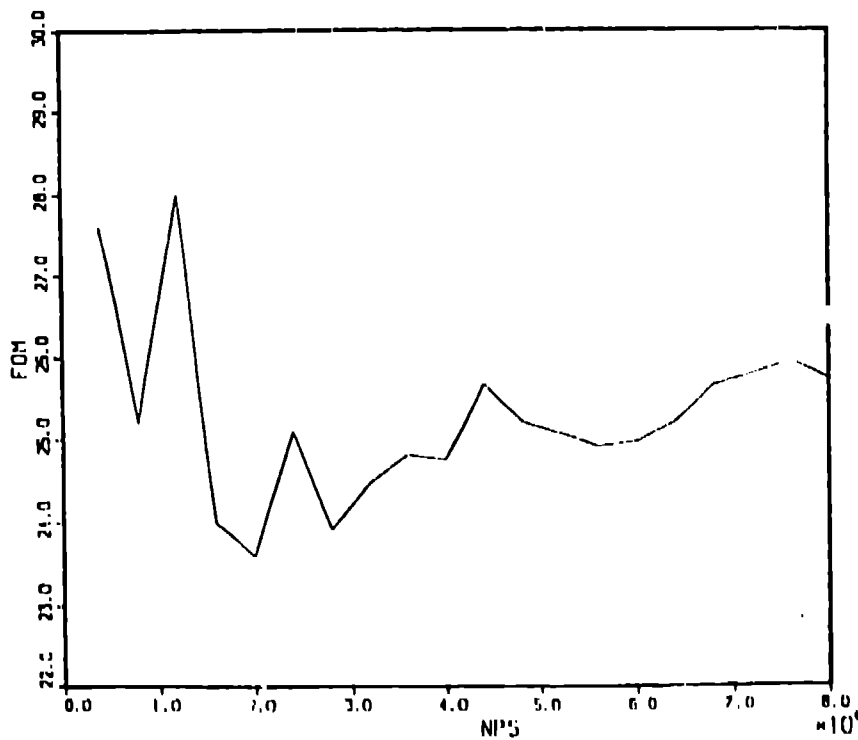
MCNP 28 03/12/82
X 03/12/82 0:43:30
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
H MULT 1
C COSINE 2
E ENERGY 117
T TIME 1
DUMP DUMP 2
--- RUNTPE

FIGURE 15
TRANSMITTED CURRENT



MCNP 20 03/12/82
X 03/12/8210:43:30
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
M MULT 1
C COSINE 2
E ENERGY 117
T TIME 1
DUMP DUMP 2
—— RUNTPE

FIGURE 16
TRANSMITTED CURRENT



MCNP 20 03/12/82
X 03/12/8210:43:30
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 2
M MULT 1
C COSINE 2
E ENERGY 117
T TIME 1
DUMP DUMP 2
----- RUNTPE

FIGURE 17

casejudy3: same as casejudy3 with irrational sources

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origin=(0.00, 0.00, 0.00)
extent=(16.00, 16.00, 16.00)

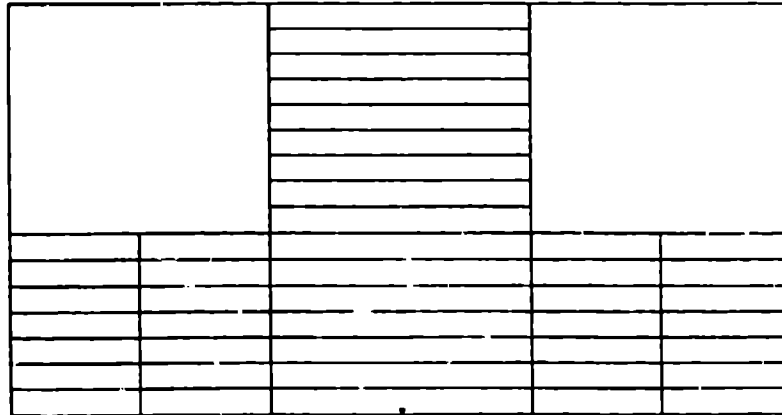
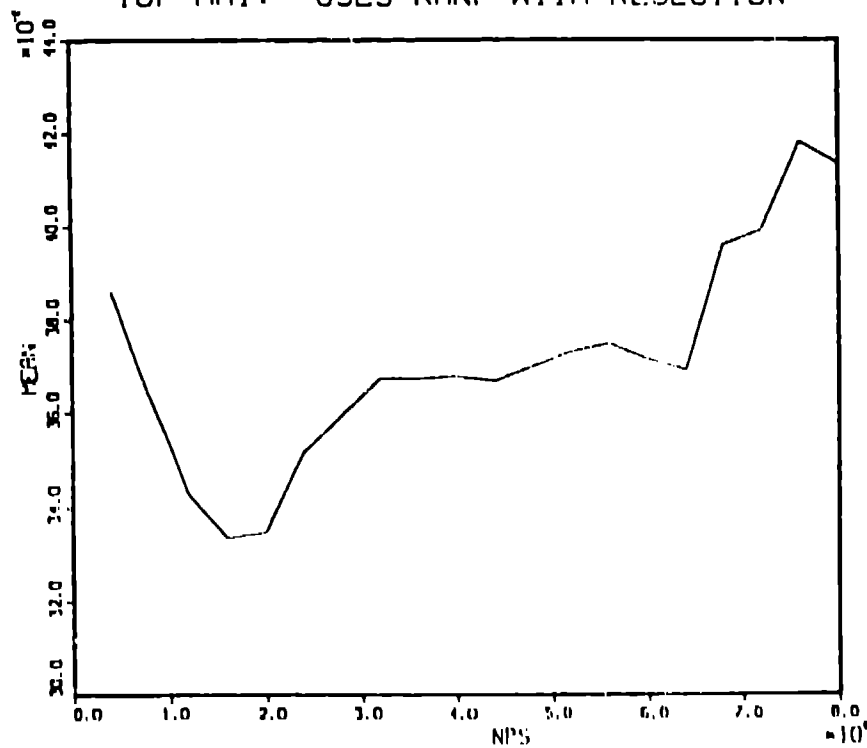


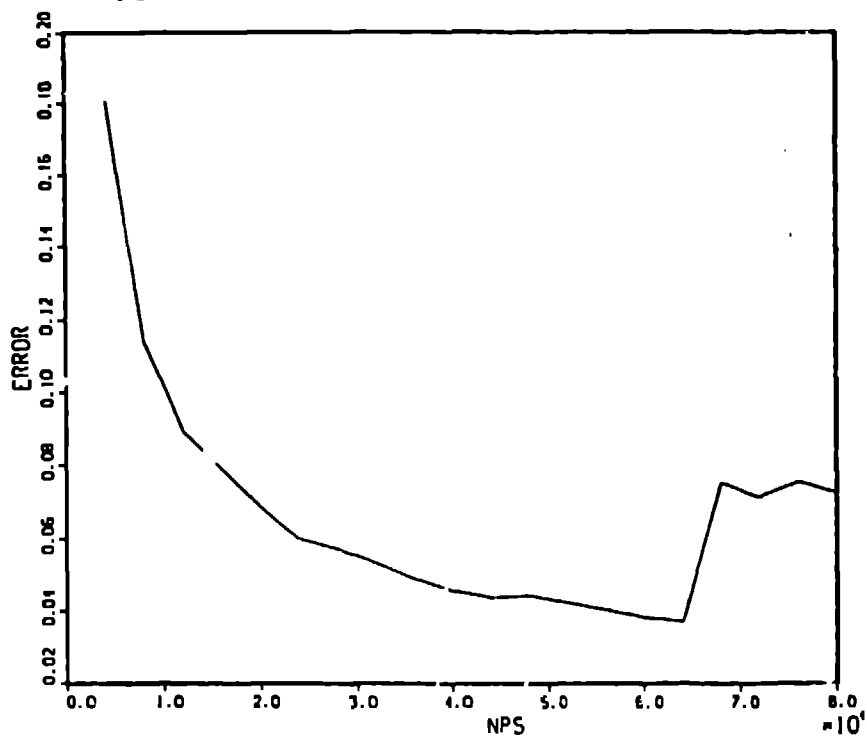
FIGURE 18

TOP HAT: USES RANF WITH REJECTION



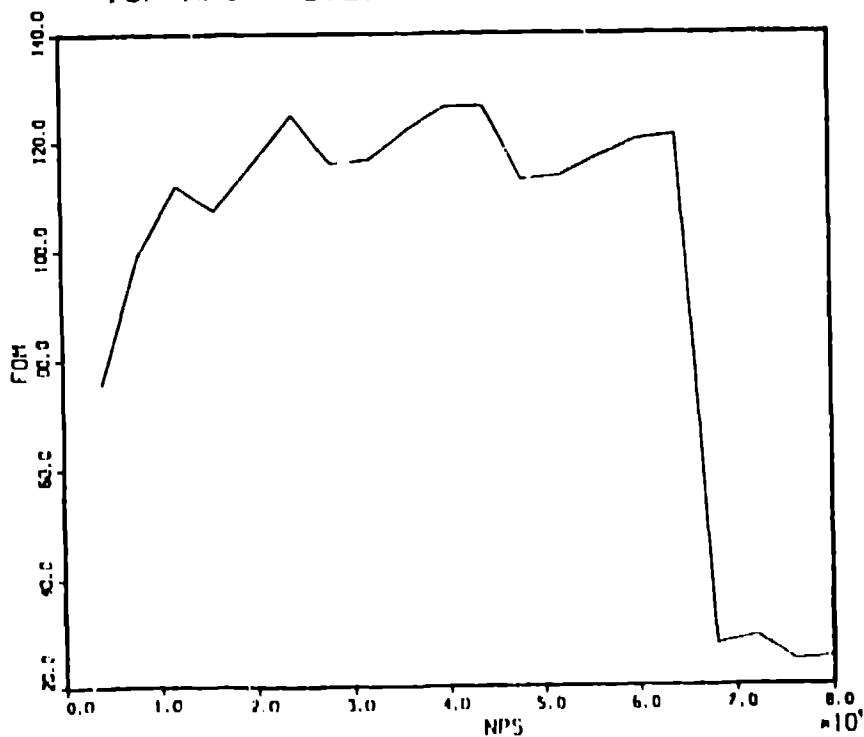
MCNP 28 03/01/02
X 03/01/02 10:17:03
TALLY= 1
NEUTRON
NPS 00001
RUNTPE= RUNR150
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 1
M MULT 1
C COSINE 1
E ENERGY 1
T TIME 1
DUMP DUMP 2
----- RUNR150

FIGURE 19
TOP HAT: USES RANF WITH REJECTION



PCNP 28 03/04/82
X 03/04/82 10:17:03
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNR150
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 1
M MULT 1
C COSINE 1
E ENERGY 1
I TIME 1
DUMP DUMP 2
----- RUNR150

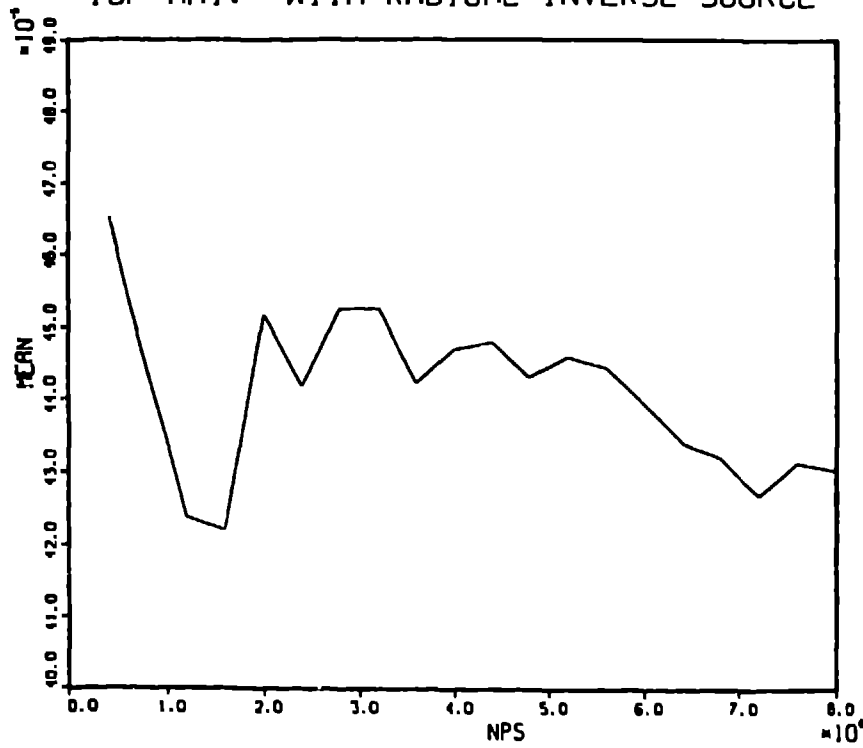
FIGURE 20
TOP HAT: USES RANF WITH REJECTION



PCNP 28 03/04/82
X 03/04/82 10:17:03
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNR150
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 1
M MULT 1
C COSINE 1
E ENERGY 1
I TIME 1
DUMP DUMP 2
----- RUNR150

FIGURE 21

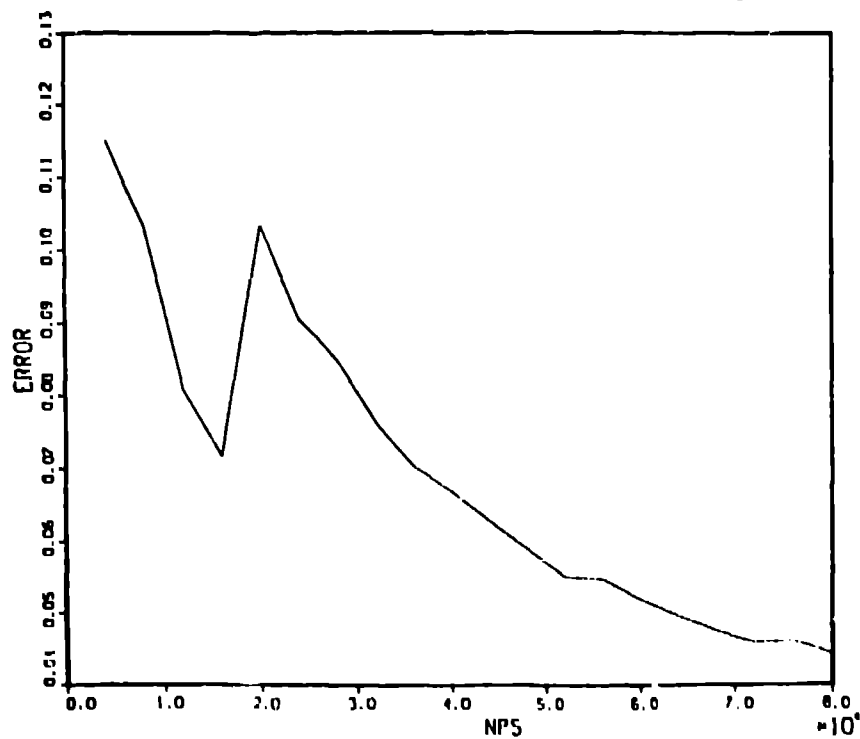
TOP HAT: WITH RADICAL INVERSE SOURCE



PCNP 28 03/15/92
 A 03/15/0210:56:11
 TALLY- 1
 NEUTRON
 NPS 80001
 RUNTPE- RUNTPE
 F SURFACE 1
 D FLAG/DIR 1
 U USER 1
 S SEGMENT 1
 M MULT 1
 C COSINE 1
 E ENERGY 1
 T TIME 1
 DUMP DUMP 2
 ——— RUNTPE

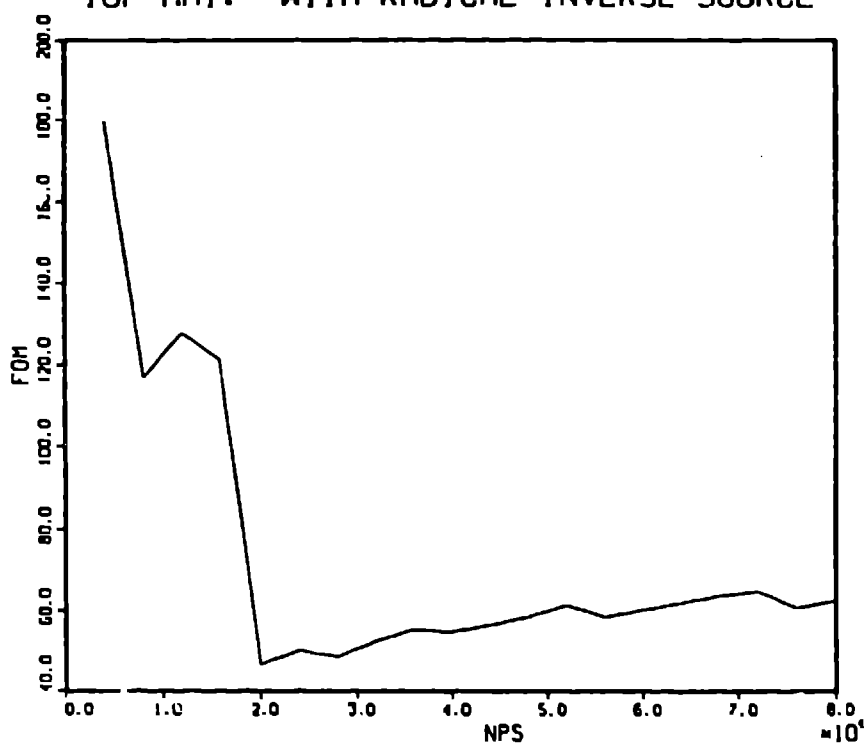
FIGURE 22

TOP HAT: WITH RADICAL INVERSE SOURCE



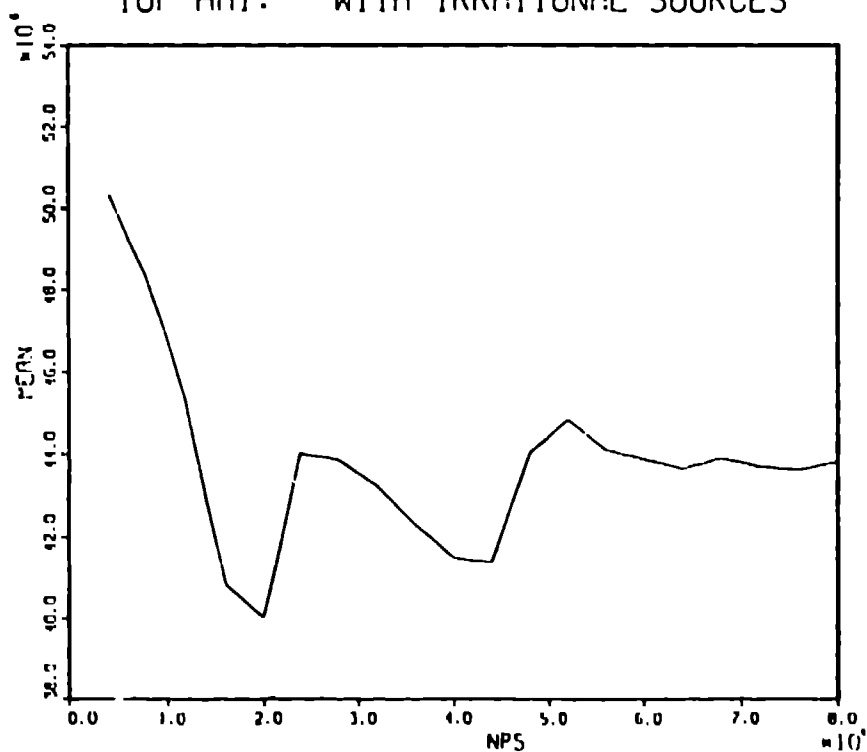
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 X 03/15/0210:56:11
 TALLY- 1
 NEUTRON
 NPS 80001
 RUNTPE- RUNTPE
 F SURFACE 1
 D FLAG/DIR 1
 U USER 1
 S SEGMENT 1
 M MULT 1
 C COSINE 1
 E ENERGY 1
 T TIME 1
 DUMP DUMP 2
 ——— RUNTPE

FIGURE 23
TOP HAT: WITH RADICAL INVERSE SOURCE



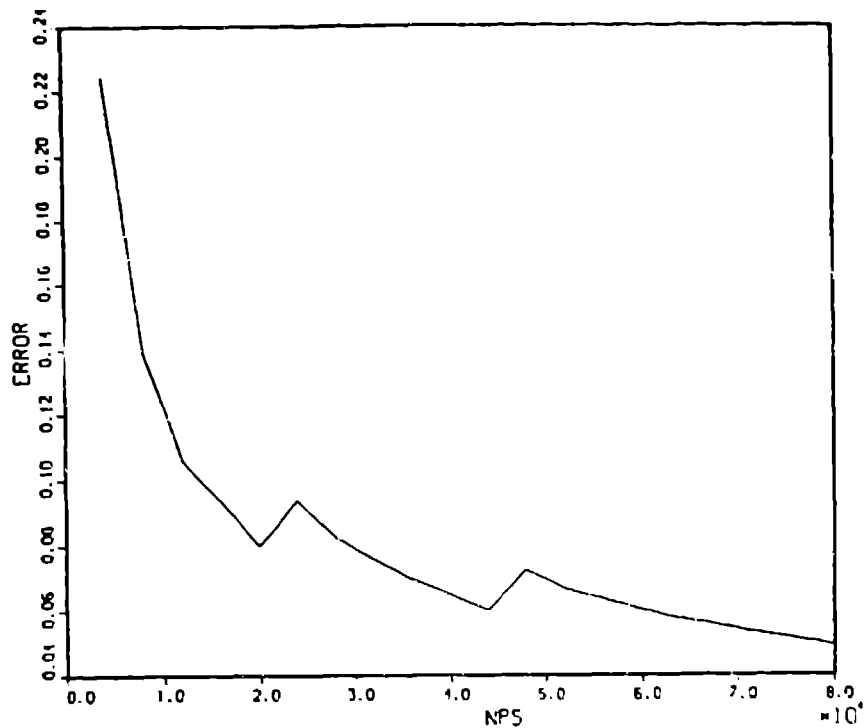
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X 03/15/8210:56:11
TALLY- 1
NEUTRON
NPS 00001
RUNTFC- RUNTFC
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 1
M MULT 1
C COSINE 1
E ENERGY 1
T TIME 1
CLMP CLMP 2
_____ RUNTFC

FIGURE 24
TOP HAT: WITH IRRATIONAL SOURCES



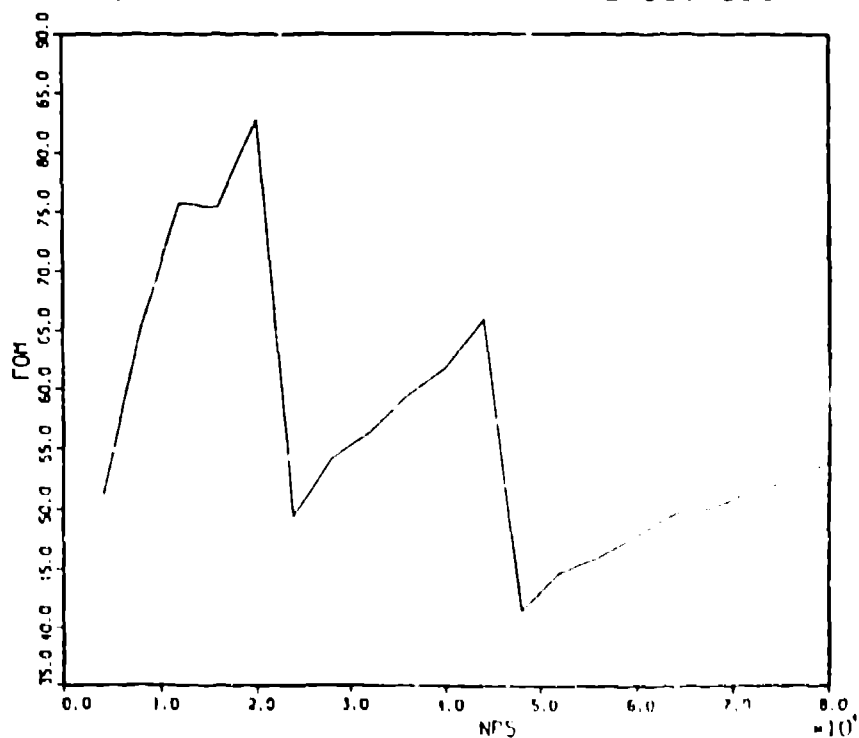
PCMP 28 03/04/82
X 03/04/8216:22:01
TALLY- 1
NEUTRON
NPS 00001
RUNTFC- RUNTFC
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 1
M MULT 1
C COSINE 1
E ENERGY 1
T TIME 1
CLMP CLMP 2

FIGURE 25
TOP HAT: WITH IRRATIONAL SOURCES



PCNP 28 03/04/82
X 03/04/82 16:22:01
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 1
H MULT 1
C COSINE 1
E ENERGY 1
I TIME 1
D

FIGURE 26
TOP HAT: WITH IRRATIONAL SOURCES



PCNP 29 03/04/82
X 03/04/82 16:22:01
TALLY- 1
NEUTRON
NPS 80001
RUNTPE- RUNTPE
F SURFACE 1
D FLAG/DIR 1
U USER 1
S SEGMENT 1
H MULT 1
C COSINE 1
E ENERGY 1
I I